Pattern formation in two-dimensional systems of rectangular particles

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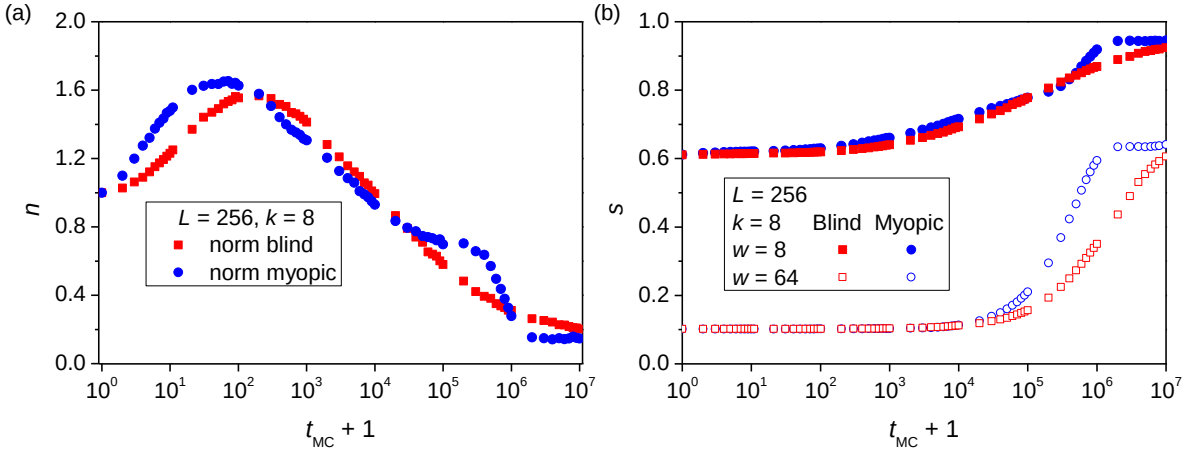
Monte Carlo simulation has been used to study reorganisation in two-dimensional systems of elongated particles. Recently, pattern formation in these systems has been reported [1–4], nevertheless, several questions are still open.

The space was assumed to be discrete, i.e., a square lattice of size $L_x \times L_y$. The simulations were performed both in square ($L_x = L_y$) and in rectangular systems ($L_x \neq L_y$). Rigid rectangular particles of size $m \times n$ lattice units were deposited onto the lattice using random sequential adsorption until a jamming state. A special attention to the case of 'needles' or k-mers, i.e., particles of size $1 \times k$, has been paid. Moreover, effect of particles shape has been studied. Two mutually perpendicular orientations of the particles were equiprobable. In the case of k-mers, the jamming state was characterised by a stack structure, i.e., the particles of the same orientation form blocks with typical size $k \times k$.

After deposition, the particles were allowed to perform a random walk. Hard-core interaction between particles was assumed, hence, any reorganisation have to be entropy-driven. Two different kinds of random walk have been studied, i.e., "blind" and "myopic" random walk rules [5]. "Blind" particle chooses the next step from among all neighbour sites. This behaviour is related to a diffusion of conventional particles, it preserves detailed balance condition [4]. "Myopic" particles are "intellectual", i.e., they choose from among all unblocked sites. This rule resembles the behaviour of particles inside active colloids. This algorithm does not preserve the detailed balance condition [4].

The normalized number of clusters, *n*, local order parameter, *s*, fraction of interspecific contacts, and mean degree of freedom of the particles have been monitored during simulations. The random walk leaded to states when particles were more free than in the initial jammed state. We calculated diffusion coefficients and found that the random walk should be considered as a subdiffusion. Examples of behavior of some quantities are presented in figure.



(a) normalized number of clusters, (b) local order parameter vs Monte Carlo steps, t_{MC}.

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